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Doping of Silicon with Phosphorus Using the $^{30}Si(p, \gamma)^{31}P$ Resonant Nuclear Reaction

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We discuss the production of phosphorus atoms in a natural silicon target when it is bombarded with an energetic proton beam, as a consequence of the $^{30}Si(p, \gamma)^{31}P$ resonant nuclear reaction. The depth concentration of phosphorus is analysed as a function of proton energy. Our calculation shows that the shape and the location of the phosphorus profile can be accurately described if the proton beam energy is properly controlled.

1. Introduction

New applications and advances in the microelectronics industry demand a considerable improvement in the production and characterization of novel device structures. Phosphorus doped silicon is widely used in very large-scale integration devices [1] or in manufacturing particle detectors [2]. Numerous studies have been devoted to predict and to understand the phosphorus concentration obtained when bombarding silicon targets with energetic phosphorus ions [3 to 8]. However, one of the main drawbacks of the above-mentioned method is that it requires high-energy phosphorus ions (of the order of or greater than 1 MeV) to implant them in the target at depths of 1 μm or deeper [9], and the direct implantation with heavy ions produces damage in the silicon matrix. These processes depend upon the mass, energy and dose of the implanted species, so one of the main aims in the direct implantation techniques is to reduce or avoid, if possible, the damage effects generated in the target [1, 10].

Recently a method to dope silicon with phosphorus was proposed [11]. The phosphorus atoms are produced inside a silicon target as a result of the $^{30}Si(p, \gamma)^{31}P$ resonant nuclear reaction, which takes place when an energetic proton beam bombards a natural silicon sample.

In Section 2 we review the fundamentals of the theory used to calculate the phosphorus concentration resulting from the $^{30}Si(p, \gamma)^{31}P$ reaction. The effects on the phosphorus concentration due to the energy of the proton beam are analysed in detail in Section 3. Finally, the conclusions are finally presented in Section 4.

2. Theoretical Model

2.1 The $^{30}Si(p, \gamma)^{31}P$ resonant nuclear reaction

An energetic proton beam bombarding a natural silicon target can induce the $^{30}Si(p, \gamma)^{31}P$ resonant nuclear reaction. By capturing a proton, the target nucleus ^{30}Si is transmutated into an excited ^{31}P nucleus, which decays from the resonance level to the ground level by emitting a γ-ray. The nuclear reaction can take place only within small energy intervals Γ_i around certain proton energies E_i (Γ_i and E_i are the resonance width and the resonance energy, respectively). Therefore, as a final result of this process, the silicon matrix becomes doped with phosphorus atoms.

For the case of isolated resonances, the dependence of the cross section for the $^{30}Si(p, \gamma)^{31}P$ resonant nuclear reaction upon the proton energy can be written using the Breit-Wigner formula [12] as

$$\sigma(E) = \frac{\pi\hbar^2}{4ME} \sum_i \frac{\Gamma_i S_i(\mathrm{p},\gamma)}{(E - E_i)^2 + \Gamma_i^2/4}\,, \tag{1}$$

where the summation includes all the nuclear resonances, M and E are the proton mass and energy, respectively, and $S_i(\mathrm{p},\gamma)$ represents the strength of each resonance. The fact that the incident (proton) and target (^{30}Si nucleus) particles have spin $\frac{1}{2}$ and 0, respectively, has been taken into account in obtaining the above expression.

We show in Fig. 1 the resonant nuclear reaction cross section according to Eq. (1), calculated using available experimental data [13] in a wide proton energy range. We can observe that there are several resonances that are quite strong and appear clearly distinct from the neighbouring resonances. In this paper we shall in particular restrict our discussion to the resonance energy $E_2 = 942$ keV, which is the strongest one and also the one most clearly separated from its nearest neighbours ($E_1 = 620.4$ keV and $E_3 = 1203.4$ keV, respectively).

Therefore, in the rest of this paper we shall limit our analysis to proton beam energies around 1 MeV. A similar discussion could be done for proton energies close to the other resonance energies.

2.2 Phosphorus depth concentration in silicon

Let us consider the case when a proton beam with a nominal initial energy E_0, distributed according to the function $g(E_0)$, bombards a semi-infinite silicon target, whose surface is located at $x = 0$. The number of phosphorus atoms produced per unit volume at the depth x, during the time interval $(t, t + \mathrm{d}t)$, is

$$Q_\mathrm{P}(x, t) = Q_\mathrm{Si}(x, t)\, \Psi(x) \tag{2}$$

with $Q_\mathrm{Si}(x, t) = n_\mathrm{Si} c(x, t)$, where n_Si is the atomic density of natural silicon, $c(x, t)$ is the abundance of ^{30}Si in natural silicon at the depth x and the time t; $\Psi(x)$ is the number of protons per unit time at the depth x, which induce the nuclear reaction.

The ^{30}Si abundance varies with the elapsed time since the start of the bombardment, according to the relation

$$\frac{\mathrm{d}Q_\mathrm{Si}(x, t)}{\mathrm{d}t} = -\,Q_\mathrm{P}(x, t)\,. \tag{3}$$

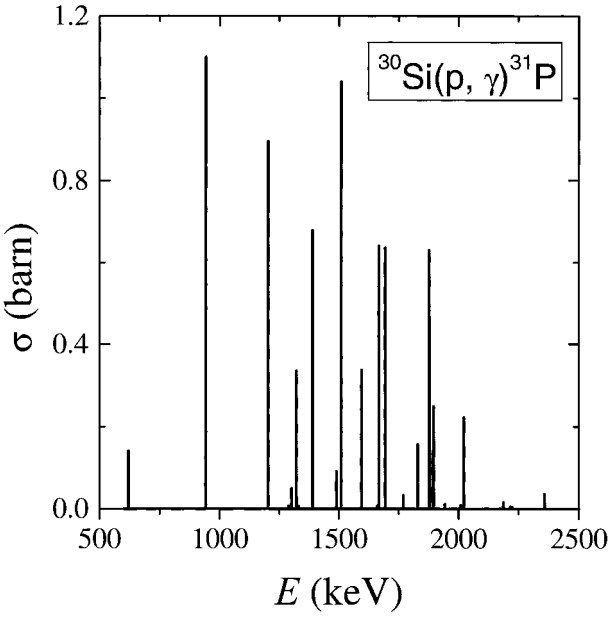

Fig. 1. Cross section corresponding to the resonant nuclear reaction ^{30}Si(p, γ)^{31}P, as a function of the proton energy. The data used in Eq. (1) were taken from Ref. [13]

Using Eq. (2) to solve the differential Eq. (3) we obtain

$$Q_{\mathrm{P}}(x,\, t) = n_{\mathrm{Si}}\, c\, \Psi(x)\, \exp\left[-\Psi(x)\, t\right], \tag{4}$$

where c is the initial abundance of ^{30}Si in a natural silicon sample [12], which does not change with the depth.

After integrating Eq. (4) from $t = 0$ to t, we obtain the number of phosphorus atoms per unit volume created at the depth x, due to the bombardment with a proton dose ϕ,

$$N_{\mathrm{P}}(x,\, \phi) = n_{\mathrm{Si}}\, c\, \{1 - \exp\left[-\phi f(x)\right]\}. \tag{5}$$

To obtain this expression we have taken into account that $\Psi(x)t = \phi f(x)$, where $f(x)$ is the fraction of protons, in a unit area transversal to the direction of the beam, which induces the nuclear reaction at the depth x. For usual doses (of the order of 10^{12} to 10^{18} protons cm^{-2}) a series expansion of the previous equation gives the approximate result

$$N_{\mathrm{P}}(x,\, \phi) \simeq n_{\mathrm{Si}}\, c\, \phi\, f(x). \tag{6}$$

On the other hand, the fraction of protons that induces the nuclear reaction at the depth x is

$$f(x) = \int \mathrm{d}E\, G[g(E_0);\, E,\, x]\, \sigma(E), \tag{7}$$

where $G[g(E_0); E, x]$ is a functional of $g(E_0)$ and a function of E and x, and it represents the distribution of protons with energy E at the depth x, corresponding to a proton beam with the initial energy distribution $g(E_0)$. It is given by

$$G[g(E_0);\, E,\, x] = \int \mathrm{d}E_0\; g(E_0)\, F(E_0 - E,\, x) \tag{8}$$

with $F(E_0 - E, x)$ being the distribution of protons that having an initial energy E_0 suffer an energy loss $(E_0 - E)$ after a path length x; $F(E_0 - E, x)$ is the Landau-Vavilov

distribution [14, 15], which we take to be of a Gaussian form

$$F(E_0 - E, x) = \frac{1}{\delta\sqrt{2\pi}} \exp\left\{-\frac{\left[(E_0 - E) - \bar{E}\right]^2}{2\delta^2}\right\}, \tag{9}$$

where $\bar{E}$ and δ represent, respectively, the mean energy loss and the fluctuation in the energy loss of a proton with initial energy E_0 after travelling a path x.

The slowing down of a proton entering a medium with initial energy E_0 until it reaches the resonance energy E_i is characterized by the stopping power S_p and the energy loss straggling Ω^2; the evaluation of these quantities at the average energy $\mathcal{E} = (E_0 + E_i)/2$ will take into account the variation of the proton energy as the proton slows down. Then $\bar{E}$ and δ are in a simple way related to these quantities by

$$\bar{E} = xS_p(\mathcal{E}), \qquad \delta^2 = x\Omega^2(\mathcal{E}). \tag{10}$$

Noting that we are dealing with very sharp resonances, we make the approximation that only those values of E contribute to the integration in Eq. (7), where the cross section has a sharp maximum, which occurs for the resonance energies, $E = E_i$. Then, from Eq. (6), we obtain that the phosphorus depth concentration after a proton dose ϕ is given by[1])

$$N_P(x, \phi) = k\, n_{Si}\, c\, \phi \sum_i G[g(E_0); E_i, x]\, \sigma(E_i)\, \Gamma_i. \tag{11}$$

The constant k comes from replacing the integral in Eq. (7) by the summation in Eq. (11), because, after numerical integration of Eq. (7) we obtain that the relationship between these is constant and approximately equal to $k = 1.57$.

The proton beam initial energy distribution $g(E_0)$ is taken to be a Gaussian centred at the nominal energy of the accelerator, $\overline{E_0}$, and with an energy spread ΔE_0:

$$g(E_0) = \frac{1}{\Delta E_0\sqrt{2\pi}} \exp\left\{-\frac{(E_0 - \overline{E_0})^2}{2(\Delta E_0)^2}\right\}. \tag{12}$$

After some algebra we obtain the depth concentration of phosphorus atoms

$$N_P(x, \phi) = k\, n_{Si}\, c\, \phi\{2\pi[(\Delta E_0)^2 + x\Omega^2(\mathcal{E})]\}^{-1/2} \times \sum_i \sigma(E_i)\, \Gamma_i \exp\left\{-\frac{1}{2}\frac{\left[\overline{E_0} - E_i - xS_p(\mathcal{E})\right]^2}{(\Delta E_0)^2 + x\Omega^2(\mathcal{E})}\right\}. \tag{13}$$

For the proton energies we are interested in this paper (≈ 1 MeV) and for not too thick targets (a few micrometers), only an isolated resonance ($E_2 = 942$ keV) will contribute to the summation over E_i in Eq. (13), as can be seen in Fig. 1. In the case of higher proton energies or thicker targets we would need to include further resonance energies in Eq. (13), because since the proton energy decreases as it slows down, resonances of lower energy can occur. However this does not affect (at least qualitatively) the main results we shall discuss in the next section.

[1]) This expression and Eq. (13) correct a misprint that appeared in Eq. (5) and Eq. (7) of Ref. [11].

2.3 Approximate calculations

Apart from the detailed discussion above, it is possible to estimate the position and width of the phosphorus profile. The distance L where the phosphorus depth concentration will be maximal depends on the nominal incident proton beam energy, $\overline{E_0}$, and on the resonance energy, E_i. Assuming a continuous slowing down of the projectile into the target, the distance L from the target surface at which a proton with incident energy $\overline{E_0}$ has the resonant energy E_i is related to the stopping power $S_{\mathrm{p}}(E)$ by

$$L = -\int_{\overline{E_0}}^{E_i} \frac{\mathrm{d}E}{S_{\mathrm{p}}(E)} \,. \tag{14}$$

In fact, L corresponds to the path travelled by the proton, not to the depth from the surface, but for the energies involved both quantities practically coincide [16, 17]. According to the available data for the proton stopping power in silicon [16, 17] we can approximate Eq. (14) by

$$L \approx \frac{\overline{E_0} - E_i}{S_{\mathrm{p}}(\mathcal{E})} \,. \tag{15}$$

We have checked that replacing Eq. (14) by Eq. (15) is a good approximation for the energies we are considering in this work.

The width of the phosphorus profile is characterized by its full width at half maximum (FWHM). It is determined by the energy spread ΔE_0 of the proton beam, the proton energy loss straggling $\Omega^2(\mathcal{E})$ due to the inelastic scattering processes and the total width Γ_i of the nuclear resonance:

$$\mathrm{FWHM} \approx \frac{\sqrt{8 \ln 2[(\Delta E_0^2) + L\Omega^2(\mathcal{E})] + \Gamma_i^2}}{S_{\mathrm{p}}(\mathcal{E})} \,. \tag{16}$$

Equations (15) and (16) allow the possibility to roughly estimate the values of L and FWHM, which characterize the phosphorus depth concentration into the silicon target. However, with this rough estimation it is not possible to calculate the maximum value of the phosphorus depth concentration.

3. Results

In this section we shall analyse the depth distribution of phosphorus atoms, Eq. (13), for representative variations of the parameters that characterize the incident proton beam.

We shall restrict our discussion to the case of a proton beam with a nominal energy $\overline{E_0} \approx 1000$ keV, and with an energy spread $\Delta E_0 \approx 20$ keV. The stopping power and the energy loss straggling for energetic ions in solids are not perfectly well defined and there are some discrepancies in the values quoted in the literature, these discrepancies being generally small for the stopping power [16, 17], but not so small for the energy loss straggling [18, 19]. In order to check the dependence of the results on the value used for S_{p}, we have considered two possible values of the silicon stopping power for protons, according to the semiempirical predictions of SRIM [20] or the dielectric formalism [21], respectively. For the energy loss straggling we use the Bohr straggling [22],

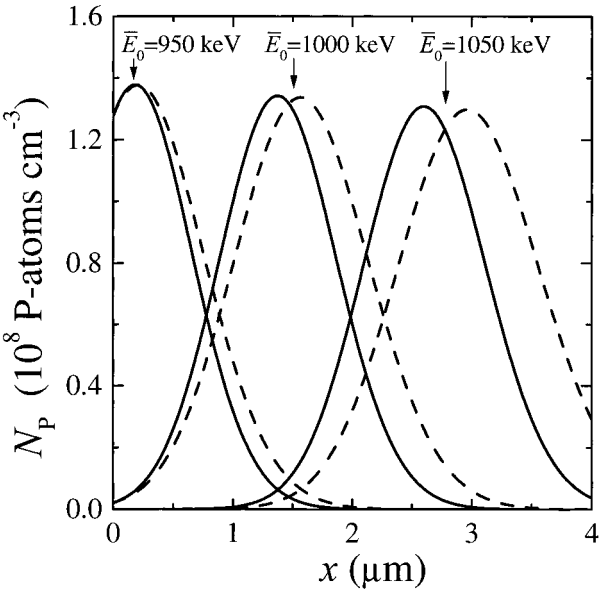

Fig. 2. Phosphorus depth concentration produced by the nuclear reaction $^{30}Si(p,\gamma)^{31}P$, for small variations around the accelerator nominal energies $\overline{E_0} = 950, 1000$ and 1050 keV. Solid and dashed lines correspond, respectively, to the results obtained with the stopping power from SRIM [20] or from the dielectric formalism [21]. The value of ΔE_0 is kept constant at 20 keV; the dose is $\phi = 10^{15}$ protons cm^{-2}

which is independent of the proton energy, and is given by $\Omega_B^2 = 4\pi Z_1^2 e^4 n_{Si} Z_2 = 1820\ \text{eV}^2/\text{Å}$, where Z_1 and Z_2 are the projectile (proton) and target (silicon) atomic numbers, respectively, and e is the electronic charge. We choose the Bohr straggling because measurements or theories for Ω^2 are scarce and Ω_B^2 is a reasonably good compromise for high proton energies. In all cases considered below, the proton dose will be 10^{15} proton cm^{-2}.

The effects of using two different values of the stopping power $S_p(\mathcal{E})$, with $\mathcal{E} = (\overline{E_0} + E_2)/2$, on the phosphorus depth distribution are shown in Fig. 2. The solid and dashed lines denote the results obtained using the stopping powers given by SRIM [20] or by the dielectric formalism [21], respectively; they are shown in Table 1. All the calculations were done with $\Delta E_0 = 20$ keV. In the energy range considered, the stopping power decreases as the proton energy increases, therefore the protons suffer the 942 keV nuclear resonant reaction further away from the target surface, and the phosphorus depth concentration shifts towards deeper regions; this is accompanied by a slight increase of the width of N_P and a small reduction of its maximum value. For each incident energy, the phosphorus profiles calculated using the stopping power provided by the dielectric formalism are slightly deeper than those obtained according to SRIM;

Table 1
Stopping power $S_p(\mathcal{E})$ of silicon for ≈1 MeV protons, evaluated at $\mathcal{E} = (\overline{E_0} + E_2)/2$

$\overline{E}_0$ (keV)	S_p(eV/Å)[a]	S_p(eV/Å)[b]
950	4.28	3.75
1000	4.21	3.69
1050	4.15	3.64

[a]) According to SRIM [20].
[b]) According to the dielectric formalism [21].

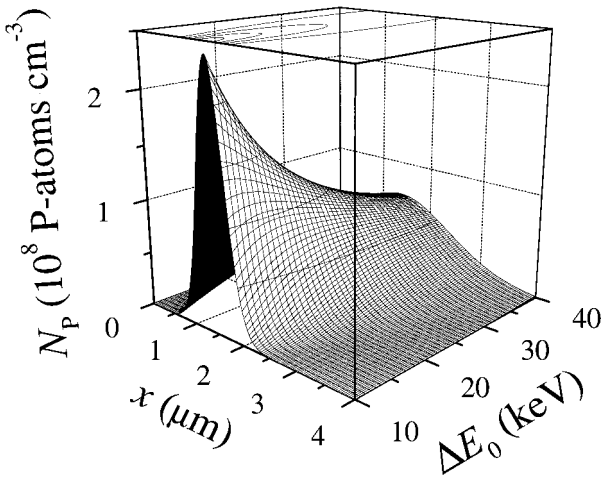

Fig. 3. Phosphorus depth concentration produced by the nuclear reaction $^{30}Si(p,\gamma)^{31}P$, for small variations around the proton energy spread ΔE_0. The initial proton energy is kept constant at $\overline{E_0} = 1000$ keV and the stopping power derived from SRIM [20] has been used. The dose is $\phi = 10^{15}$ protons cm^{-2}

this is due to the lower values of S_p by the first method as compared with the latter, as can be seen in Table 1.

We have also checked that there are no significant effects on N_P for a variation of $\pm 25\%$ in Ω^2 around the Bohr straggling value, Ω_B^2. The reason for this small effect is that $L\Omega_B^2 \ll (\Delta E_0)^2$, therefore its influence on the phosphorus concentration is negligible.

In Fig. 3 we illustrate the influence of the initial proton energy beam spread ΔE_0 on the phosphorous depth distribution. By keeping the initial proton beam energy constant at $\overline{E_0} = 1000$, we have varied the initial energy spread in the range $\Delta E_0 = 10$ to 40 keV. Although the maximum value of N_P decreases as ΔE_0 increases, its position does not vary appreciably. The decrease of the maximum value of N_P is accompanied by a broadening of the phosphorus depth concentration, but the total number of phosphorus produced in the silicon target does not vary significantly (the area under each section of Fig. 3 with ΔE_0 constant is practically the same). For a given value of $\overline{E_0}$, sharper phosphorus profiles are obtained with smaller values of ΔE_0. Therefore, according to the results shown in Figs. 2 and 3, the main parameters to control the depth concentration of the phosphorus atoms inside the silicon target are the initial energy, $\overline{E_0}$, and the energy spread, ΔE_0, of the proton beam, which determine the position and the width of the phosphorus profile.

For the case in which $\overline{E_0} = 1000$ keV and $\Delta E_0 = 20$ keV, the values of L obtained from Eq. (15) using $S_p(\mathcal{E})$ from SRIM [20] or from the dielectric formalism [21] are 1.38 and 1.57 μm, respectively. Using Eq. (16) we obtain that FWHM $= 1.15$ and 1.32 μm for the two values of $S_p(\mathcal{E})$, where we have taken $\Omega^2(\mathcal{E}) = \Omega_B^2$, according to our previous discussion. These estimations are in excellent agreement with the results shown in Fig. 2.

4. Conclusions

We have shown that phosphorus atoms can be produced in a silicon sample when it is bombarded with a MeV proton beam, due to the $^{30}Si(p,\gamma)^{31}P$ resonant nuclear reaction. This method offers an alternative procedure to the usual direct implantation of

phosphorus. It has the advantage of reducing the damage produced in the sample, since a light projectile is used instead of a medium-mass one. However, high proton doses should be needed to attain conventional phosphorus concentrations, therefore the proton dose must be carefully controlled in order to produce detectable effects, but to avoid blistering effects in the silicon target.

The depth of the dopant distribution is mainly governed by the nominal energy of the incident proton beam, $\overline{E_0}$, which determines the stopping power and energy loss straggling of the target, and also by the energy and width of the nearest resonance to $\overline{E_0}$, such that $E_i < \overline{E_0}$. The calculated phosphorus depth distributions have an almost Gaussian shape with a broad width, compared to the narrow and asymmetric distributions obtained by direct phosphorus ion bombardment. It is worth to noting that a variation of a few percent of the proton beam energy, $\overline{E_0}$, affects in an appreciable manner the position of the phosphorus concentration but not its width.

From Figs. 2 and 3 (and their respective captions) it can be seen that it is possible to choose the appropriate initial conditions of the proton beam to obtain a desired doping profile (sharper or broader, closer to or further away from the target surface ...).

The results presented in this paper refer to individual resonances. If a thick silicon target is irradiated by protons with sufficiently high energy, there is the possibility to create simultaneously several dopant layers at fixed relative distances, depending upon the resonance energies. With the formalism developed in this work it is also possible to calculate the time needed to create a doped layer with a given concentration. These two aspects will be discussed in detail in a forthcoming paper. The method developed in this work can also be applied to the study of other resonant nuclear reactions, which could take place in ion bombarded solids.

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